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QUANTUM CHEMICAL INVESTIGATIONS OF THE MECHANISM OF CATIONIC PO--ETC(U)

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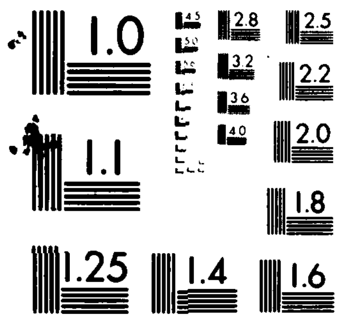

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Report Number ONR-NR093064-TR2

SUMMARY

ANNUAL REPORT

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QUANTUM CHEMICAL INVESTIGATIONS OF THE MECHANISM OF CATIONIC POLYMERIZATION

and

THEORETICAL PREDICTION OF CRYSTAL DENSITIES

and

DECOMPOSITION PATHWAYS OF ENERGETIC MOLECULES

Joyce J. Kaufman, Principal Investigator
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Baltimore, Maryland 21218

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II. Development of theoretical procedures for prediction of crystal structures and densities.

III. Ab-initio quantum chemical MODPOT/VRDDO/MERGE calculations on nitro-explosives.

IV. Decomposition pathways of energetic compounds.

Quantum chemical calculations on the large molecules have been carried out with our own programs which also incorporate several desirable options for calculations on large molecules.

I. In the research on part I of this project we are carrying out ab-initio quantum chemical calculations and generating electrostatic molecular potential maps for cationic polymerization.

There are two major steps in the polymerization of cyclic ethers, the initiation step proportional to basicity and ring strain of the cyclic ether and the propagation step, attributed by experimentalists to the electrophilicity of the propagating carbocation. Electrostatic molecular potential contour maps generated from our ab-initio MODPOT/VRDDO calculations on the cyclic ethers prove to be reliable indicators of the relative basicities of these ethers and their propensity to undergo cationic polymerization. We are continuing such calculations both on the cyclic ethers themselves and on the proton attack on these ethers to get a coherent overview of the initiation problem. These maps also indicate good copolymer coordinates. These maps now form a semi-quantitative guide to the ease of polymerizability of energetic cyclic ethers.

The opening of the ring is influenced by ring strain. We also developed a theoretical index which is indicative of ring strain.

We derived several theoretical indices which should be indicative of electrophilicity and carried out these calculations on oxetane with various energetic substituent groups. By all the criteria the carbocation from dinitrooxetane should be the most electrophilic. However, since oxetane, which has the least electrophilic carbocation, polymerizes easily under conventional Lewis acid catalysis using a BF_3 catalyst and dinitrooxetane does not polymerize under those conditions, but only much more difficultly using a PF_5 catalyst, it is the initiation step which dominates the ease of polymerizability - not the propagation step.

II. We have derived and coded a program for the prediction of crystal structures and densities. The program is based on calculating the various intermolecular interaction terms from ab-initio SCF wave functions and the dispersion term and then using these to construct the crystal structure. Tests are now underway.

III. Ab-initio SCF quantum chemical calculations have been carried out on all of the large nitroexplosive molecules whose crystal sturctures had been determined experimentally and on a number of nitropolyhedranes. The wave functions for a total of 61 such molecules have been calculated to date.

IV. Preliminary ab-initio SCF, GVB and MC-SCF/CI calculations were carried out for the dissociation of HNO_2 and SCF and GVB calculations were carried out for the dissociation of CH_3NO_2 as prototypes of R--NO_2 decomposition. Multideterminant reference states turn out to be necessary to describe HNO_2 and CH_3NO_2 even at their equilibrium geometries and even larger multideterminant reference states are necessary to describe dissociation properly.

QUANTUM CHEMICAL INVESTIGATIONS OF THE MECHANISM OF CATIONIC POLYMERIZATION AND THEORETICAL PREDICTION OF CRYSTAL DENSITIES AND DECOMPOSITION PATHWAYS OF ENERGETIC MOLECULES

Joyce J. Kaufman, Principal Investigator

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I. Ab-Initio Quantum Chemical Investigations of the Mechanism of Cationic Polymerization

There are several steps in the cationic polymerization mechanism of cyclic ethers. First is initiation by attack of a proton or Lewis acid on the ring oxygen, then opening of the ring at the C-O bond and propagation by attack of the protonated species on the next molecule of cyclic ether.

The propensity for polymerization had been demonstrated experimentally by Aoki, et al., to be influenced by the basicities and ring strains of the cyclic ethers. Electrostatic molecular potential contour maps generated from our ab-initio MODPOT/VRDDO calculations on the cyclic ethers prove to be reliable indicators of the relative basicities of these ethers and their propensity to undergo cationic polymerization. We are continuing such calculations both on the cyclic ethers themselves and on the proton attack on these ethers to get a coherent overview of the initiation problem.

The opening of the ring is influenced by the ring strain. We have derived a semi-quantitative theoretical index which allows us to compare relative ring strains not only among differently substituted cyclic ethers with rings with the same number of ring atoms but also between rings with different numbers of atoms. The influence of substituents on the relative ring strains in rings with the same number of ring atoms is neglibible compared to the differences in ring strain in rings with different numbers of ring atoms.

The propensity for propagation of a protonated species was suggested by experimental polymer chemists as being influenced by the "electrophilicity" of the protonated species or by the positive charge localized at the end carbon. Quantum chemical calculations on the protonated ring-opened species indicated that neither the "electrophilicity" as reflected in electrostatic molecular potential contour maps nor the positive charge

localized on the end carbon differed very much as a function of substituent on the oxetane (4-membered) ring at the 3 position.* On the other hand, "electrophilicity" as reflected in unoccupied molecular orbital energies was significantly different.* Thus, since unsubstituted oxetane (the most basic, with the least electrophilic protonated ring-opened species) does undergo cationic polymerization easily with conventional Lewis acid BF_3 catalyst and 3,3-dinitrooxetane (the least basic species, with the most electrophilic protonated ring-opened species) only undergoes cationic polymerization with difficulty with a Lewis acid PF_5 catalyst, it is the initiation step which is dominant in preventing the cationic polymerization of 3,3-dinitrooxetane under conventional Lewis acid catalyst conditions.

For the new energetic cyclic ethers, when there is experimental kinetic data against which to compare, our theoretical indices are expected to enable a semi-quantitative ranking of propensity to polymerize and will indicate which of the steps dominates.

Technical manuscripts are being written up on various aspects of this research. One manuscript has already appeared and several more have been accepted for publication and are in press. Presentations of this research on cationic polymerization have been given at a number of national and international meetings. Our paper on "Ab-Initio MODPOT/VRDDO/MERGE Calculations and Electrostatic Molecular Potential Contour Maps for Mechanism of Cationic Polymerization"[Δ] presented at the International Sanibel Symposium on Atomic, Molecular and Solid State Theory, Palm Coast, Florida, March 1981 was awarded first place as the best paper presented at that meeting.

Molecular electrostatic potential contour maps have been calculated for a number of additional energetic cyclic ethers, protonated cyclic ethers and the ring opened protonated carbocations after optimization of their geometries. Calculations are also being carried out at present on additional energetic cyclic ethers and attack of protons on these to optimize their geometries prior to calculating their molecular electrostatic potential contour maps.

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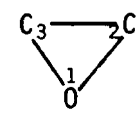
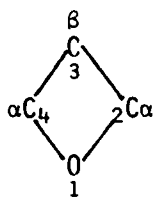
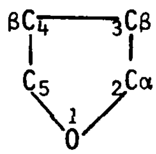
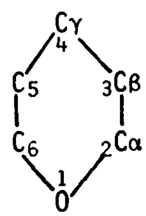
* See Tables following page 7.

Δ A preprint copy of that manuscript is enclosed with this technical report.

CALCULATIONAL STATUS

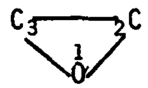
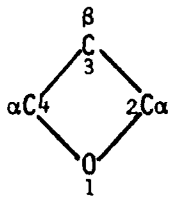
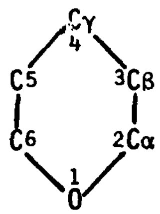
Geometry optimizations being carried out

PARENT RING SYSTEM	MOLECULE
	2-Ethyloxirane (N-Nitro-N-methylamino)methyloxirane (2-Fluoro-2,2-dinitroethoxy)methyloxirane (1-Fluoro-1,1-dinitroeth-2-oxy)oxirane (2-Azido-2,2-dinitroeth-2-oxy)oxirane
	2,3-Bis(azidomethyl)oxetane 3-Methyl-3-(1,1-dinitroprop-3-oxy)oxetane
	3-(2,2-Dinitropropyl)oxolane 2-Methyloxolane 2-Ethyloxolane Oxolan-2-ol
	2-Ethyloxane

CALCULATIONAL STATUS

Electrostatic Molecular Potential Contour Maps

<u>Cyclic ethers</u>

PARENT RING SYSTEM	MOLECULE
	2-(Azidomethyl)oxirane 2-Methylazidooxirane 2-Methyloxirane
	2-Methyloxetane 2-Ethyloxetane 3-Fluorooxetane 3-Nitrooxetane
	3,3-Bis(azidomethyl)oxetane BAMO for a number of different choices for starting geometries to be optimized
	3-(2,2-Dinitropropyl)oxetane 3-(2-Fluoro-2,2-dinitroethoxymethyl)-3-methyloxetane 3-(2-Fluoro-2,2-dinitroeth-1-oxy)oxetane Oxetan-2-ol
	2-Methyloxane Oxan-2-ol

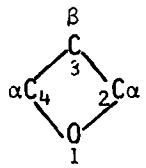
(continued on next page)

CALCULATIONAL STATUS

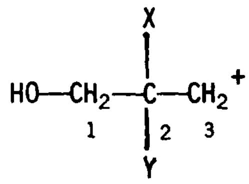
Electrostatic Molecular Potential Contour Maps (Continued)

<u>Protonated</u>

<u>Oxetane</u>



<u>Propanolyl positive ion</u>



Note that the standard convention for numbering is now different between the two species. These calculations were run in each case both for the tetrahedral and planar arrangement of atoms around carbon 3

	X	Y
oxetane	H	H
3-azidooxetane	N_3	H
3-fluorooxetane	F	H
3-nitrooxetane	NO_2	H
3-fluoro-3-nitrooxetane	F	NO_2
3,3-dinitrooxetane	NO_2	NO_2
3,3-bis(azidomethyl)oxetane	CH_2N_3	CH_2N_3

For some of these protonated oxetanes further geometry optimizations are being carried out since these are difficultly convergent calculations.

ESTIMATE OF COMPARATIVE RING STRAIN

RING TOTAL OVERLAP POPULATIONS/ # ATOMS IN RING

CYCLIC ETHERS

			Protonated	
Ring Size	B $\Sigma TOP/n$	B + NB $\Sigma TOP/n$	B $\Sigma TOP/n$	B + NB $\Sigma TOP/n$
3- OXIRANE	.3705	.3705	.3461	.3461
4- OXETANE	.5690	.4180	.5239	.4016
5- OXOLANE	.5974	.4805	.5500	
6- OXANE	.6189	.4622	.5750	

EXPERIMENTAL

Stability (Comparative)

$$3- < 4- < 5- \underset{?}{\lesseqgtr} 6-$$

B = Bonded Ring Atoms

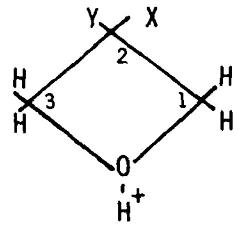
B + N = Bonded + Non-Bonded Ring Atoms

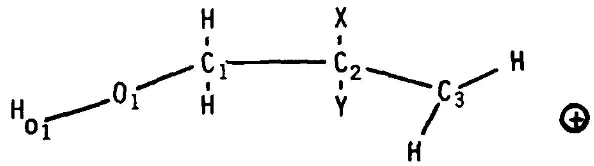
2-X-2-Y-OXETANES PROTONATED

2-X-2-Y-PROPAN-1-OL CARBOCATIONS

AB-INITIO MODPOT/VRDDO/MERGE

ENERGIES AND GROSS ATOMIC POPULATIONS





Non-Standard Numbering for Comparison
to Propan-1-ol's

X	Y	Geom	Energy(a.u.)	GAP's C_2	O_1	H_{O_1}
H	H	t	-35.733807	4.023	6.536	0.607
		p	-35.746961	4.013	6.535	0.607
		prot	-35.811184	4.193	6.449	0.500
F	H	t	-59.030070	4.026	6.535	0.601
		p	-59.041364	4.019	6.534	0.601
NO_2	H	t	-75.988651	4.000	6.534	0.595
		p	-75.999395	3.995	6.533	0.595
NO_2	NO_2	t	-116.227994	3.975	6.532	0.586
		p	-116.237806	3.975	6.531	0.586
		prot	-116.289185	4.173	6.444	0.478
F	NO_2	t	-99.280104	3.995	6.533	0.588
		p	-99.290046	3.993	6.533	0.589
		prot	-99.371903	4.197	6.441	0.478
H	N_3	t				
		p	-63.915196	4.152	6.537	0.605
		prot	-63.991020	4.187	6.446	0.497

t = tetrahedral arrangement around C_3

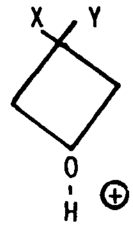
p = planar arrangement around C_3

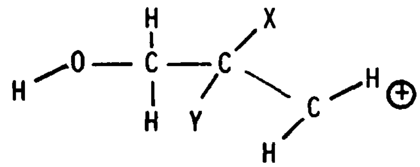
prot = protonated oxetane ring

PROTONATED OXETANES AND CORRESPONDING RING-OPENED PROPAN-1-OL CARBOCATIONS

AB-INITIO MODPOT/VRDDO/MERGE

ORBITAL ENERGIES (a.u.) HOMO AND 3 LUMO's





X	Y	Geom	HOMO	1st LUMO	2nd LUMO	3rd LUMO
H	H	prot	-0.723853	-0.058360	+0.064974	+0.197895
		t	-0.645764	-0.273129	+0.127244	+0.136488
		p	-0.645804	-0.270947	+0.109784	+0.220072
H	N_3	prot	-0.571073	-0.065085	-0.040998	-0.019661
		t				
		p	-0.599636	-0.281461	-0.075991	-0.051255
F	NO_2	prot	-0.598276	-0.134358	-0.104127	+0.017668
		t	-0.624579	-0.328564	-0.158542	+0.063826
		p	-0.620561	-0.325604	-0.155066	+0.042692
NO_2	NO_2	prot	-0.601068	-0.162007	-0.126256	-0.121584
		t	-0.636031	-0.337011	-0.188754	-0.157300
		p	-0.632170	-0.334192	-0.184982	-0.153796

II. Development of Theoretical Procedures for Prediction of Crystal Structures and Densities

Detonation velocity is influenced by crystal density. For hypothetical energetic molecules suggested for synthesis it is of interest to try to predict in advance at least the upper limit of their crystal densities.

For this we have formulated and implemented methods for partitioning the calculated ab-initio intermolecular interaction energies into their separate components and fitting these components separately to potential functions. Comparison of the electrostatic contribution to the molecular interaction energy calculated from partitioning of the ab-initio SCF interaction energy with that calculated by the customary atomic monopole-atomic monopole expression indicated that only about 10-20% of the electrostatic interaction energy came from the atomic monopole-atomic monopole contribution and to calculate the full electrostatic contribution to intermolecular interaction energies from the atomic charges on two (or more) molecules it is necessary to include higher atomic multipole contributions and the programs for these have been coded and added to the programs. We have also coded routines for fitting the various intermolecular interaction energy terms to functional forms and for minimization of the calculated total crystal energy.

We have meshed in the strategy for the overall symmetry operation transformations necessary to generate the coordinates of all molecules in the unit cell and in any specified number of shells of unit cells around the primary unit cell. The coding for specific symmetry transformations for the particular crystal symmetries in which various explosive molecules are observed to crystallize has been included explicitly. The specific transformations for any other desired crystal symmetries can be included as found necessary.* The entire code is together and being tested.

The preliminary testing will be on smaller molecules whose crystal structures are known since for the tests we will carry out from about 40 to several hundred ab-initio SCF calculations for the molecular pairs partitioned into the various intermolecular interaction terms to check the reliability of the various functional forms for each type of energy component.

As a prelude to testing the method for known nitroexplosive crystals we carried out ab-initio MODPOT/VRDDO/MERGE calculations on all of the energetic nitrocompounds (cyclic nitramines, nitroaromatics and miscellaneous compounds) for which crystal structures have been determined. These are described in the next section.

* Credit for the crystal symmetry portion is due to Dr. Alfred Lowrey, Naval Research Laboratory, who is working with us collaboratively on the project as a fellow-by-courtesy of The Johns Hopkins University.

III. Ab-Initio Quantum Chemical MODPOT/VRDDO/MERGE Calculations on Nitroexplosives.

Ab-initio MODPOT/VRDDO/MERGE calculations have been carried out for all of the nitroexplosives for which crystal structures have been determined experimentally plus for a number of new and some hypothetical polyhedrane nitroexplosives. These calculations were the necessary first step for calculating the ab-initio MODPOT/VRDDO/MERGE SCF calculations for various conformations of the dimers and trimers of these nitroexplosives in order to perform the energy decomposition of these latter SCF wave functions to obtain the magnitudes of the various types of interaction energies to use as input for calculating the crystal energies. These ab-initio MODPOT/VRDDO/MERGE SCF calculations on the nitroexplosive molecules themselves are also the necessary first step for calculations of molecular decomposition at beyond the SCF Hartree-Fock level. As described in more detail in the following section (IV), we discovered on carrying out ab-initio SCF, GVB (Generalized Valence Bond) and MC-SCF/CI (Multiconfiguration SCF/Configuration Interaction) calculations on HNO_2 and SCF and GVB calculations on CH_3NO_2 as prototype $R\text{-}NO_2$ compounds that these $R\text{-}NO_2$ compounds do not have simple single determinant ground states. Even at their equilibrium geometries these $R\text{-}NO_2$ compounds have 2-configuration ground states. We are in the process of comparing the occupied and virtual molecular orbital character of these large nitroexplosives with those of HNO_2 and CH_3NO_2 to ascertain the probabilities that these large nitroexplosives might also have 2-configuration ground states (or multi-configuration ground states if there is more than one NO_2 group in the molecule).

The calculations for some of these molecules (especially the polynitropolyhedranes) were difficult to converge. We were able to obtain convergence for these molecules using special extrapolation and damping techniques which we had written.

The question had arisen as to the effect that substitution of nitrogroups would have on the strengths of the various C-C bonds in the polyhedranes. Adding nitrogroups to cubane affects different bonds in the cubane structures differently. Depending on the position of substitution and the geometrical conformation, various C-C bonds in the cubane skeleton can be either strengthened or weakened. The same holds true for various C-C bonds in nitroadamantanes and for various C-C and C-N bonds in nitroazaadamantanes. To get an indication of whether substitution of nitrogroups would strengthen or weaken the polyhedrane skeleton we have done some preliminary investigations using a theoretical index we had derived several years ago for heterocyclic explosives, the concept of a skeletal molecular total overlap population (MTOP). The skeletal MTOP for the unsubstituted cubane is smaller in magnitude

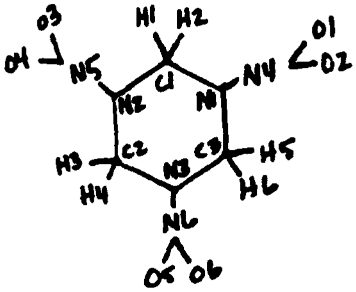
than for nitrosubstituted cubanes and the skeletal MTOP for the unsubstituted adamantane or azaadamantanes is smaller in magnitude than for the nitrosubstituted compounds. There are also further subtle differences depending on the positions of substitution and geometrical conformations. Thus, for the systems we have investigated so far apparently the effect of nitrosubstitution is to strengthen the polyhedrane skeleton. This concept will be explored in more depth.

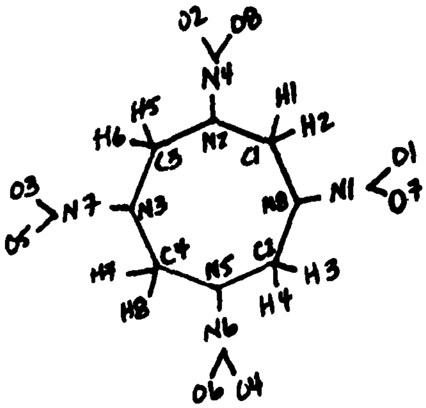
Calculations have been run on a total of 61 molecules and for different geometrical conformations. The molecules for which these calculations have been performed, their structures and computational characteristics are listed on the following pages. These molecules include saturated nitroheterocyclics (such as the nitramines RDX and HMX), nitroaromatics (with various combinations of substituents including the aminonitrobenzenes),nitrocubanes, nitroadamantanes, nitroazaadamantanes, and other types of nitrocompounds.

NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBE	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
HEXAHYDRO-1,3,5-TRINITRO-1,3,5-TRIAZINE (RDX) $C_3H_6N_6O_6$	66	833,905	779.95	547.18	14≠
				742.60	19*
OCTAHYDRO-1,3,5,7-TETRANITRO-1,3,5,7-TETRAZINE (δHMX) $C_4H_8N_8O_8$	88	934,680	1565.67	1429.16	19*





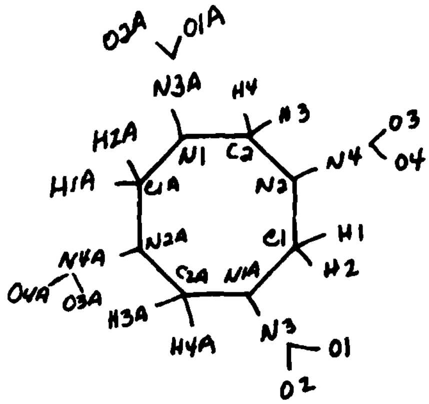
≠ 5×10^{-5} A.U. CONV.

* 1×10^{-6} A.U. CONV.

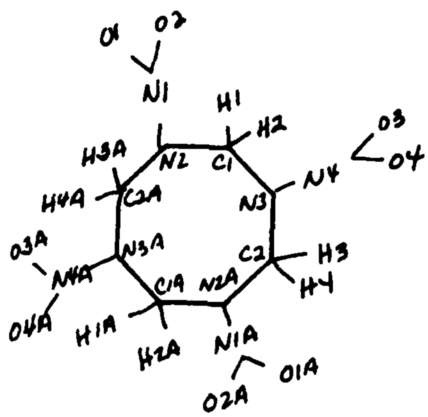
NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBF	#2E INT	TIMING(SECS) 2E INT	SCF	ITNS
OCTAHYDRO-1,3,5,7-TETRANITRO-1,3,5,7-TETRAZINE (αHMX) $C_4H_8N_8O_8$	88	982,406	1690.85	1258.58	17*



MOLECULE	NBF	#2E INT	TIMING(SECS) 2E INT	SCF	ITNS
OCTAHYDRO-1,3,5,7-TETRANITRO-1,2,5,7-TETRAZINE (βHMX)	88	1,046,595	1688.56	1392.64	17*



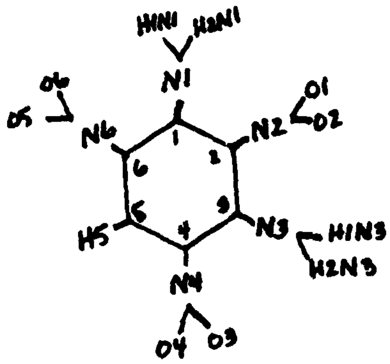
*1×10^{-6} A.U. CONV.

NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

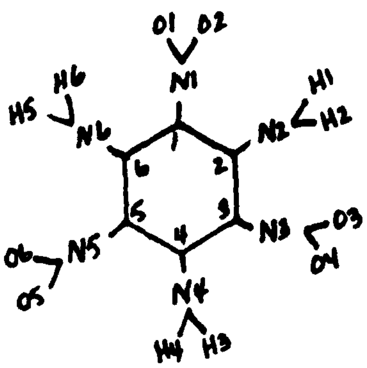
MOLECULE	NBF	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
1,3-DIAMINO-2,4,6-TRINITROBENZENE (DATB)	73	442,985	923.35	631.63	17 ≠
				1040.33	28*

$C_6H_5N_5O_6$



MOLECULE	NBF	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
1,3,5-TRIAMINO-2,4,6-TRINITROBENZENE (TATB)	78	542,795	1147.69	738.65	16 ≠
				1061.81	23*

$C_6H_6N_6O_6$

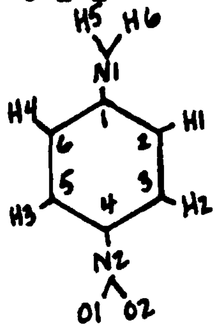
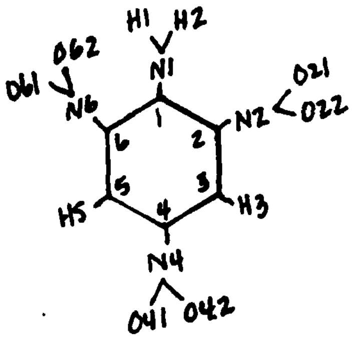
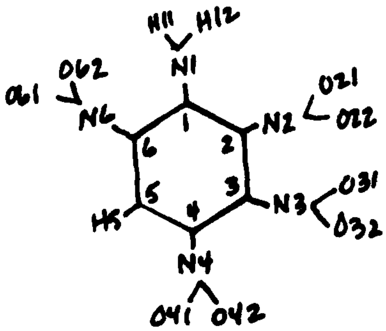


≠ 5×10^{-5} A.U. CONV.

* 1×10^{-6} A.U. CONV.

NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

			TIMING (SECS)		
MOLECULE	NBF	#2E INT	2E INT	SCF	ITNS
4-NITROANILINE	46	154,893	320.32	127.32	10≠
$C_6H_6N_2O_2$				216.44	17*
					
2,4,6-TRINITROANILINE	68	389,057	766.75	424.35	13≠
$C_6H_4N_4O_6$				685.48	21*
					
2,3,4,6-TETRANITRO-ANILINE	79	598,750	1135.05	653.74	13≠
				1056.05	21*
$C_6H_3N_5O_8$					
					

≠ 5×10^{-5} A.U. CONV.

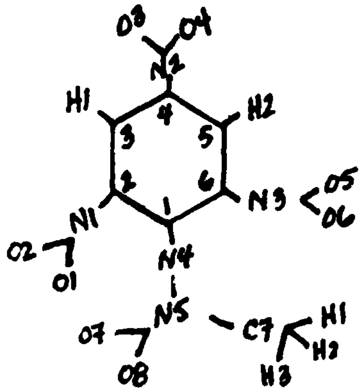
* 1×10^{-6} A.U. CONV.

NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

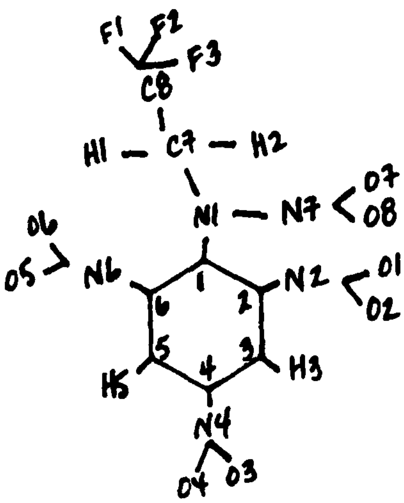
MOLECULE	NBE	#2E INT	2E INT	TIMING (SECS) SCF	ITNS
N-METHYL-N,2,4,6-TETRANITROANILINE (TETRYL)	85	893,087	1368.63	990.83	14≠
				1344.69	19*

$C_7H_5N_5O_8$



MOLECULE	NBE	#2E INT	2E INT	SCF	ITNS
N(β, β, β-TRIFLUORETHYL)-N,2,4,6-TETRANITRO-ANILINE	100	1,007,993	1892.39	1545.54	18≠
				2661.76	31*

$C_8H_4N_5O_8F_3$

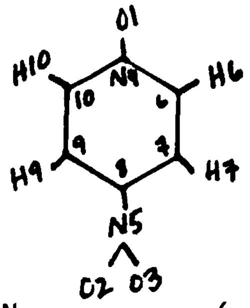
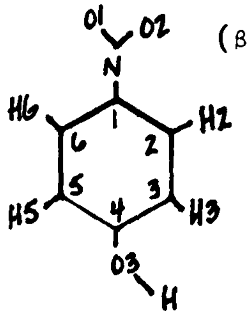
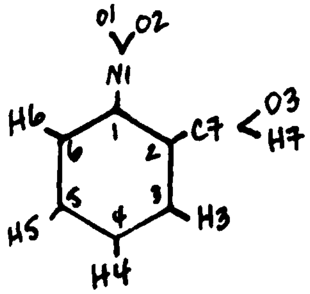


≠ 5×10^{-5} A.U. CONV.

* 1×10^{-6} A.U. CONV.

NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

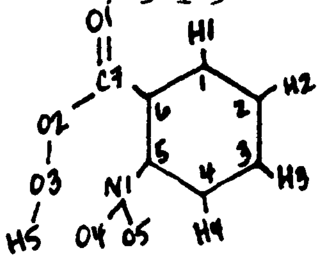
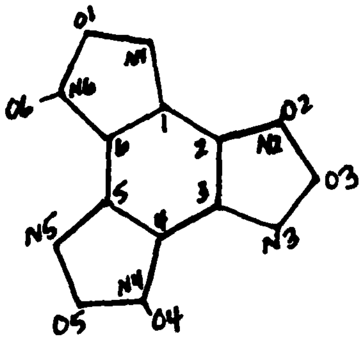
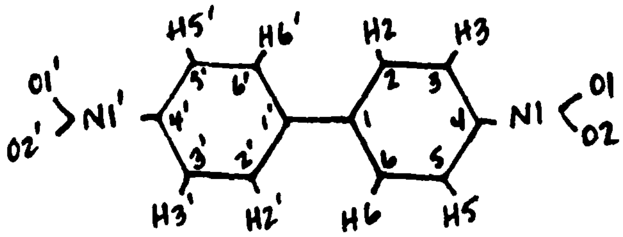
MOLECULE	NBF	#2E INT	2E INT	TIMING (SECS) SCF	ITNS
4-NITROPYRIDINE-N-OXIDE	44	116,864	276.01	158.40	16 ≠
				247.49	25*
$C_5H_4N_1O_3$					
					
P-NITROPHENOL (α)	45	146,445	294.90	145.06	12 ≠
$C_6H_5N_1O_3$				205.51	17*
(β)	45	143,923	297.96	120.96	10 ≠
				205.63	17*
					
O-NITROBENZALDEHYDE	49	215,286	374.65	254.55	15 ≠
$C_7H_5N_1O_3$				356.37	21*
					

≠ 5×10^{-5} A.U. CONV.

* 1×10^{-6} A.U. CONV.

NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBF	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
O-NITROPEROXYBENZOIC	57	283,960	497.18	343.45	15 ≠
$C_7H_5N_1O_5$				549.52	24*
					
BENZOTRIFUROXAN	72	454,853	987.62	693.26	18 ≠
$C_6N_6O_6$				962.87	25*
					
4,4'-DINITRODIPHENYL	80	629,251	1159.87	1037.93	20 ≠
$C_{12}H_8N_2O_4$				1401.21	27*
					

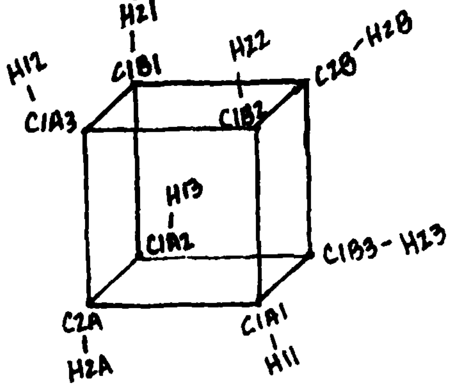
≠ 5×10^{-5} A.U. CONV.

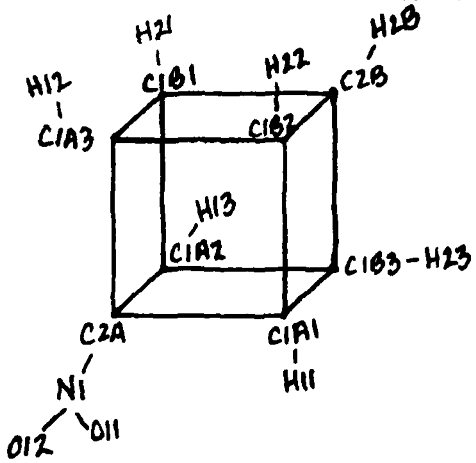
* 1×10^{-6} A.U. CONV.

NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE		NBF	#2E INT	2E INT	SCF	ITNS
				TIMING (SECS)		
CUBANE FLEISCHER STRUCTURE C_8H_8		40	269,104	366.34	175.10	10*
NITROCUBANE APEX STRUCTURE $C_8H_7NO_2$	ECLIPSED	51	398,868	595.66	357.38	13*
	STAGGERED	51	419,025	596.28	425.16	15*



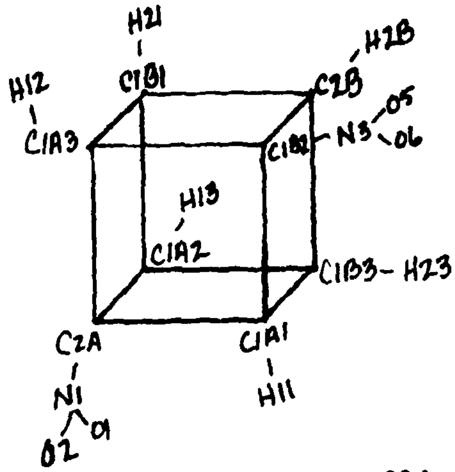


*1 x 10^{-6} A.U. CONV.

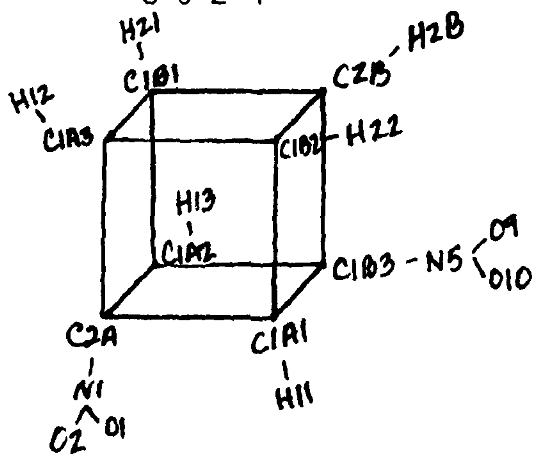
NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBF	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
DINITROCUBANE ON C2A AND C1B2 $C_8H_6N_2O_4$	62	692,708	983.89	1678.46	36*



MOLECULE	NBF	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
DINITROCUBANE ON C2A AND C1B3 $C_8H_5N_2O_4$	62	678,472	977.69	1731.83	37*

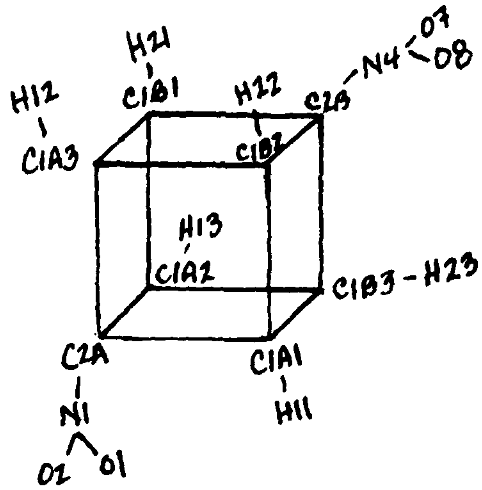


* 1 x 10^{-6} A.U. CONV.

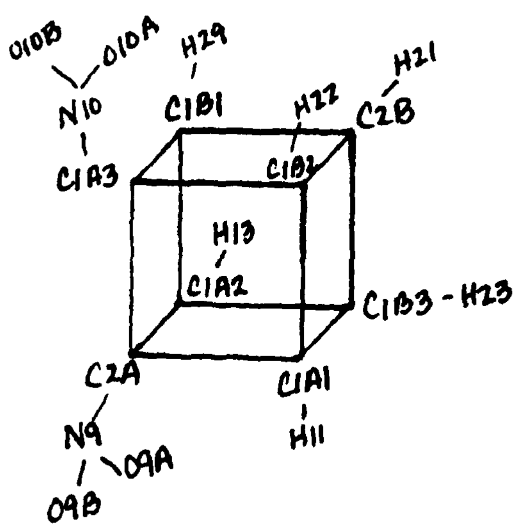
NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBF	#2E INT	2E INT	TIMING (SECS) SCF	ITNS
DINITROCUBANE ON C2A AND C2B $C_8H_6N_2O_4$	62	549,773	972.94	1650.20	37*



DINITROCUBANE ON C1A3 AND C2A $C_8H_6N_2O_4$	62	634,844	899.83	1009.12	23*

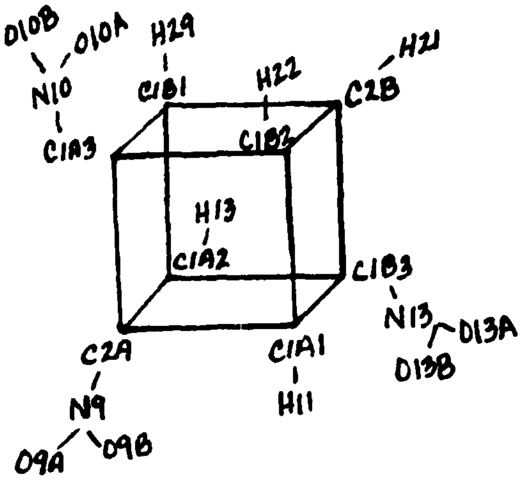


*1 x 10^{-6} A.U. CONV.

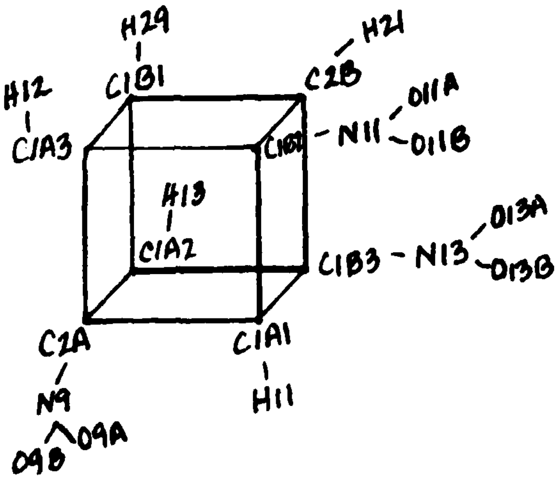
NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBF	#2E INT	2E INT	TIMING (SECS) SCF	ITNS
1,2,5-TRINITROCUBANE $C_8H_5N_3O_6$	73	856,357	1262.02	1286.11	21*



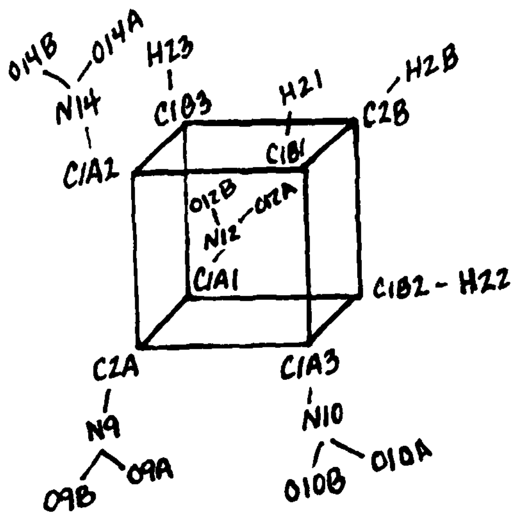
MOLECULE	NBF	#2E INT	2E INT	TIMING (SECS) SCF	ITNS
1,3,5-TRINITROCUBANE $C_8H_5N_3O_6$	73	858,682	1261.84	1282.38	21*



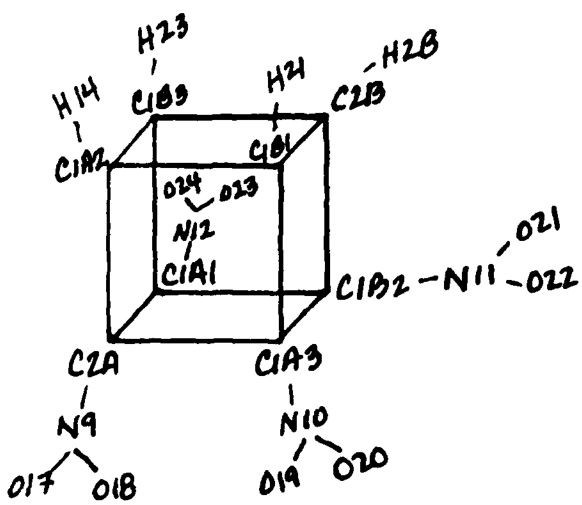
* 1×10^{-6} A.U. CONV.

NITROEXPLOSIVES

		Ab-Initio, MODPOT/VRDDO		Timing (secs)	
MOLECULE	NBE	#2E INT	2E INT	SCF	ITNS
1,2,4,6-Tetranitrocubane $C_8H_4N_4O_8$	84	1,157,701	1797.38	3324.84	40*



1,2,3,4-Tetranitrocubane $C_8H_4N_4O_8$	84	1,221,725	1874.57	2213.63	25*

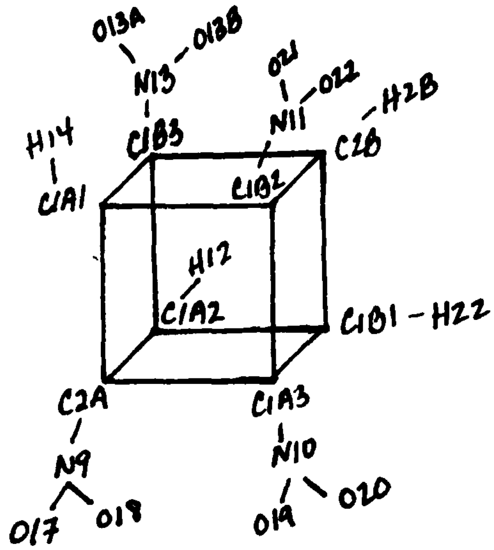


* 1 x 10^{-6} A.U. Conv.

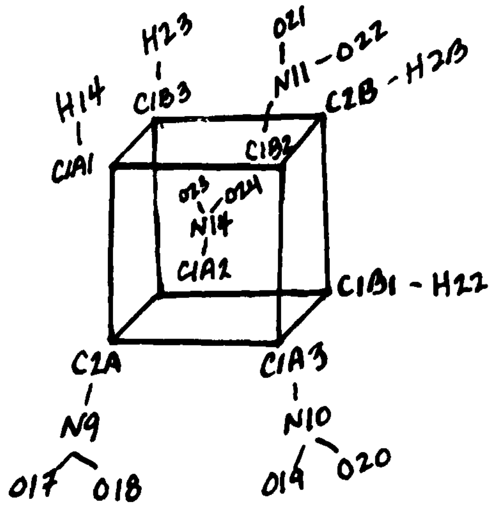
NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBE	#2E INT	2E INT	TIMING (SECS) SCF	ITNS
1,2,3,5-TETRANITROCUBANE $C_8H_4N_4O_8$	84	120,941	1825.10	2181.79	25*



MOLECULE	NBE	#2E INT	2E INT	TIMING (SECS) SCF	ITNS
1,2,3,6-TETRANITROCUBANE $C_8H_4N_4O_8$	84	1,373,694	1892.73	2217.93	25*



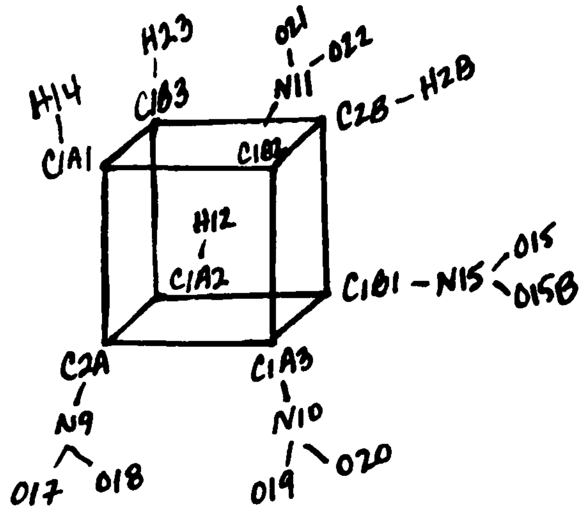
* 1 x 10^{-6} A.U. CONV.

NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

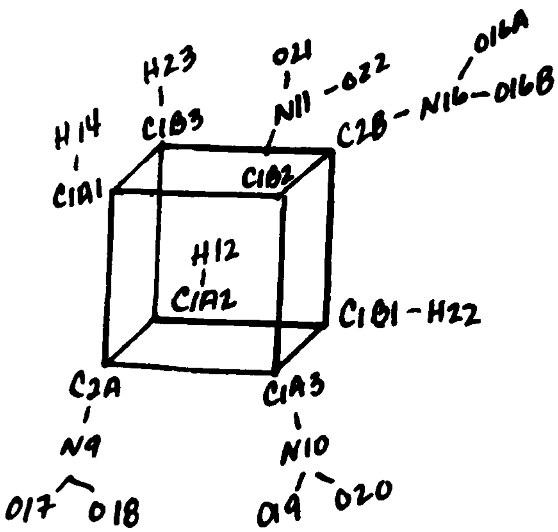
MOLECULE	NBF	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
1,2,3,7-TETRANITROCUBANE	84	1,347,287	1834.72	2182.71	25*

$C_8H_4N_4O_8$



1,2,3,8-TETRANITROCUBANE	84	1,356,319	1868.69	2195.10	25*

$C_8H_4N_4O_8$

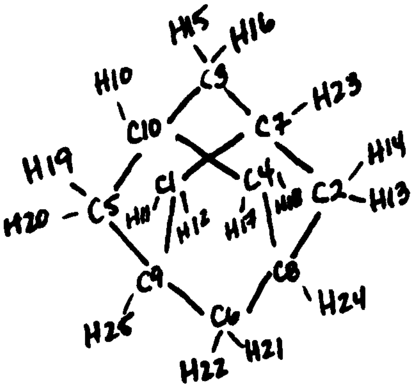


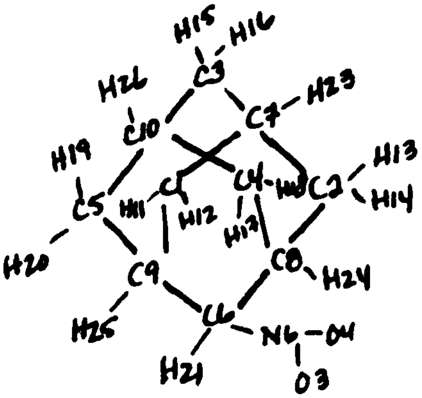
* 1×10^{-6} A.U. CONV.

NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBE	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
ADAMANTANE $C_{10}H_{16}$	56	649,528	1004.94	332.29	7*
NITROADAMANTANE, SECONDARY CARBON $C_{10}H_{15}NO_2$	67	962,892	1479.84	1533.22	22*



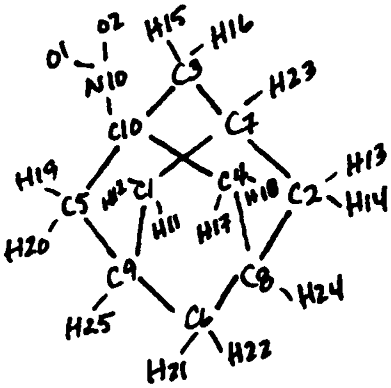


* 1 x 10^{-6} A.U. CONV.

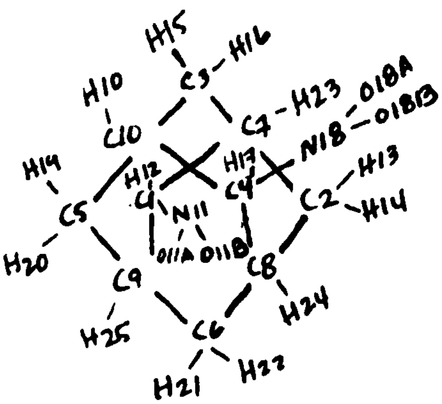
NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBF	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
NITROADAMANTANE, TERTIARY CARBON $C_{10}H_{15}NO_2$	67	1,014,762	1507.27	1003.25	15*



MOLECULE	NBF	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
1,4-DINITROADAMANTANE $C_{10}H_{14}N_2O_4$	78	1,361,395	2020.49	1385.26	15*

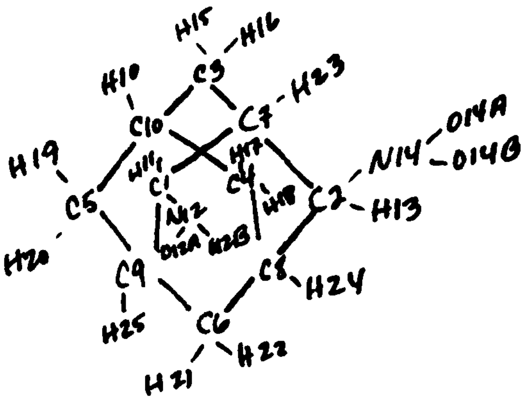


*1 x 10^{-6} A.U. CONV.

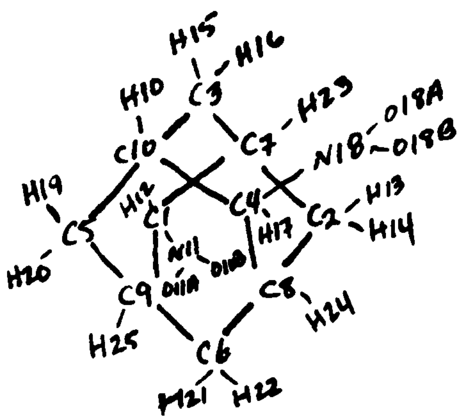
NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBF	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
1,2-DINITROADAMANTANE $C_{10}H_{14}N_2O_4$	78	356,400	1994.10	1310.78	14*



MOLECULE	NBF	#2E INT	2E INT	SCF	ITNS
1,4-DINITROADAMANTANE $C_{10}H_{14}N_2O_4$	78	1,361,395	2020.49	1385.26	15*

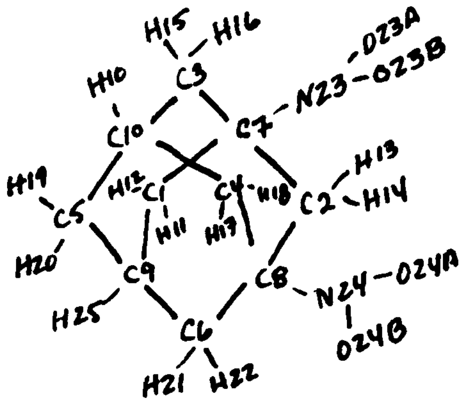


$^{*}1 \times 10^{-6}$ A.U. CONV.

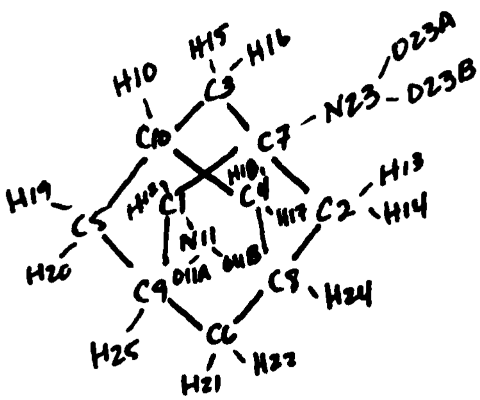
NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

			TIMING (SECS)		
MOLECULE	NBE	#2E INT	2E INT	SCF	ITNS
7,8-DINITROADAMANTANE	78	1,279,906	1843.97	1814.39	21*
$C_{10}H_{14}N_2O_4$					



1,7-DINITROADAMANTANE	78	1,378,340	1991.32	1931.72	21*
$C_{10}H_{14}N_2O_4$					

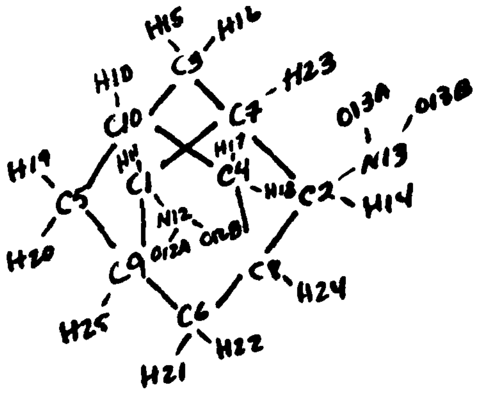


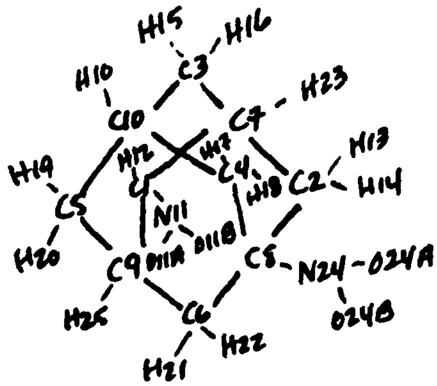
*1 x 10^{-6} A.U. CONV.

NITROEXPLOSIVES

Ab-Initio, MODPOT/VRDDO

MOLECULE	NBF	#2E INT	TIMING(SECS) 2E INT	TIMING(SECS) SCF	ITNS
1,2-Dinitroadamantane (E,A) $C_{10}H_{14}N_2O_4$	78	1,376,766	1995.79	2272.87	25*
1,8-Dinitroadamantane (A,E) $C_{10}H_{14}N_2O_4$	78	1,328,614	1919.65	1367.15	21*





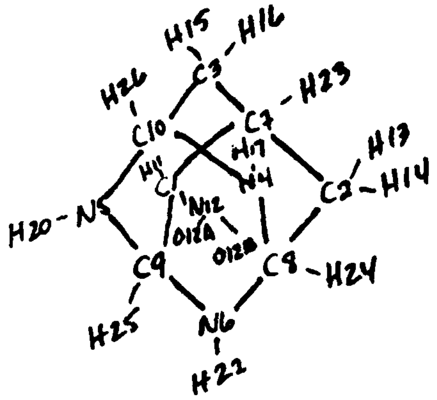
*1 x 10^{-6} A.U. Conv.

NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBE	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
1-NITRO-4,5,6-TRIAZAADAMANTANE (E)	64	814,630	1148.51	1326.88	24*

$C_7H_{12}N_{14}O_2$

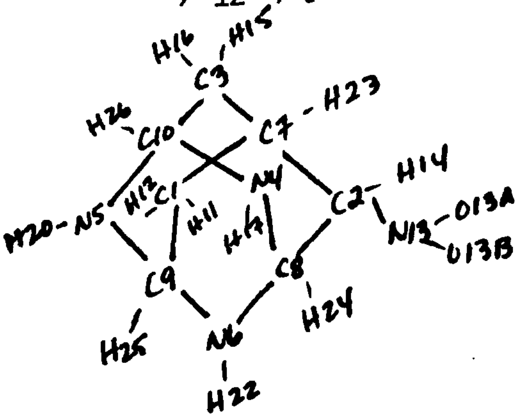


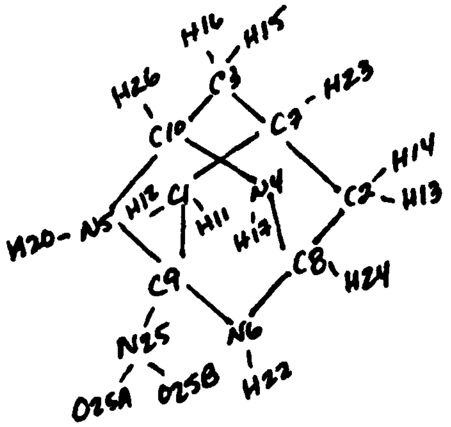
*1 x 10^{-6} A.U. CONV.

NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBF	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
2-NITRO-4,5,6-TRIAZAADAMANTANE (A) $C_7H_{12}N_4O_6$	64	797,853	1148.54	827.02	15*
9-NITRO-4,5,6-TRIAZAADAMANTANE (E) $C_7H_{12}N_4O_6$	64	759,029	1102.16	792.57	15*



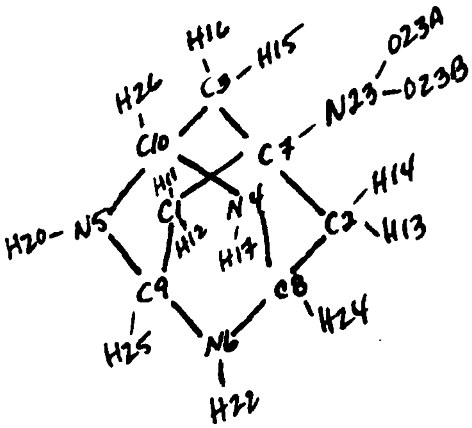


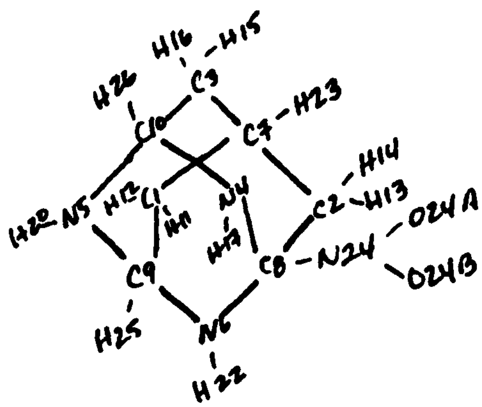
*1 x 10^{-6} A.U. CONV.

NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBF	#2E INT	2E INT	TIMING (SECS) SCF	ITNS
7-NITRO-4,5,6,-TRIAZAADAMANTANE (E) $C_7H_{12}N_4O_2$	64	796,578	1131.00	813.93	15*
8-NITRO-4,5,6-TRIAZAADAMANTANE (E) $C_7H_{12}N_4O_2$	64	761,083	1093.97	1050.07	20*



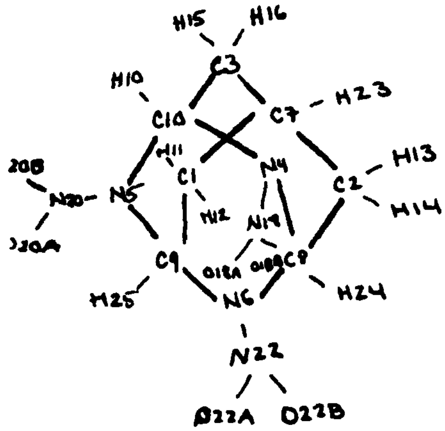


* 1×10^{-6} A.U. CONV.

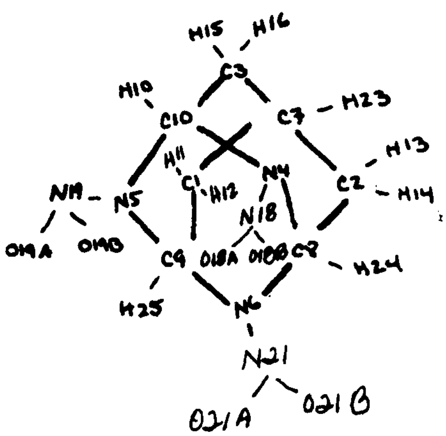
NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBF	#2E INT	2E INT	SCF	ITNS
4,5,6-TRINITRO-4,5,6-TRIAZAADAMANTANE (A,E,E) $C_7H_{10}N_6O_8$	86	1,713,704	2516.13	1589.11	14*



MOLECULE	NBF	#2E INT	2E INT	SCF	ITNS
4,5,6-TRINITRO-4,5,6-TRIAZAADAMANTANE (A,A,A) $C_7H_{10}N_6O_8$	86	1,372,581	2076.55	3264.39	34*

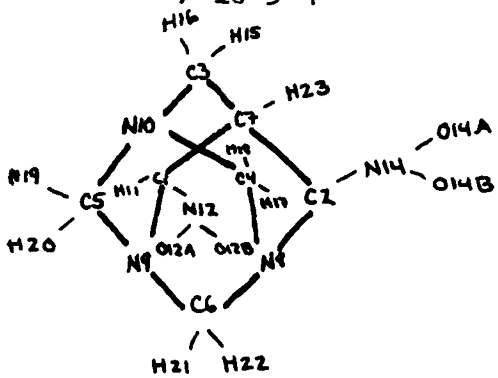


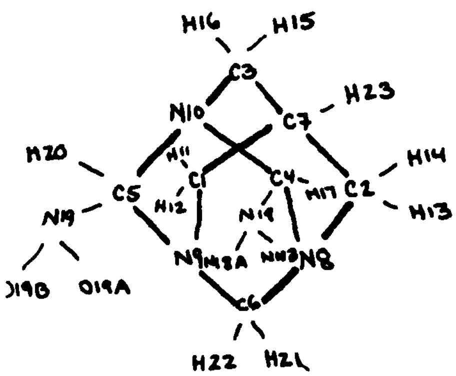
*1×10^{-6} A.U. CONV.

NITROEXPLOSIVES

Ab-Initio, MODPOT/VRDDO

MOLECULE	NBE	#2E INT	TIMING (SECS) 2E INT	TIMING (SECS) SCF	ITNS
1,2-Dinitro-8,9,10-TRIAZAADAMANTANE (E,A) $C_7H_{10}N_5O_4$	75	1,117,715	1619.25	1594.88	21*
4,5-Dinitro-8,9,10-TRIAZAADAMANTANE (A,A) $C_7H_{10}N_5O_4$	75	1,082,738	1582.56	1562.26	21*



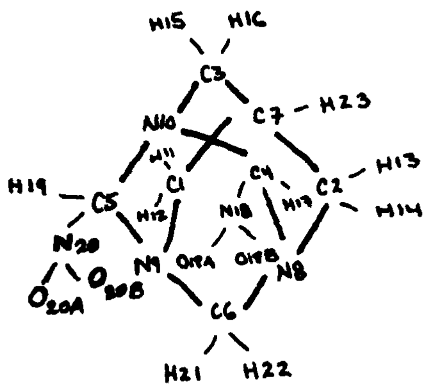


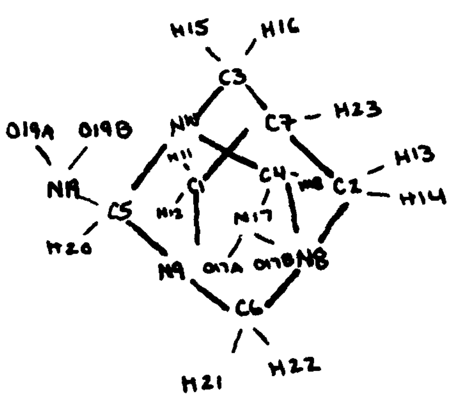
*1 x 10^{-6} A.U. Conv.

NITROEXPLOSIVES

Ab-Initio, MODPOT/VRDDO

MOLECULE	NBF	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
4,5-Dinitro-8,9,10-TRIAZAADAMANTANE (A,E) $C_7H_{12}N_5O_4$	75	1,160,795	1695.32	2939.63	38*
4,5-Dinitro-8,9,10-TRIAZAADAMANTANE (E,A) $C_7H_{11}N_5O_4$	75	1,085,605	1584.23	1875.80	25*



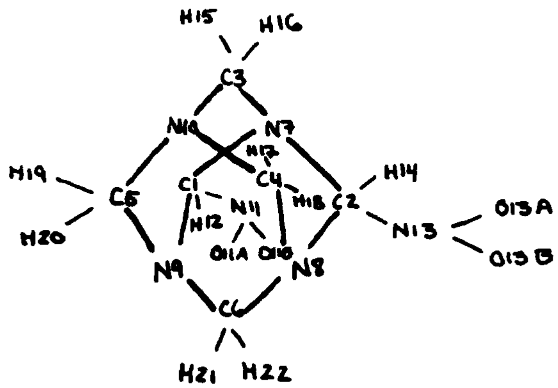


*1 x 10^{-6} A.U. Conv.

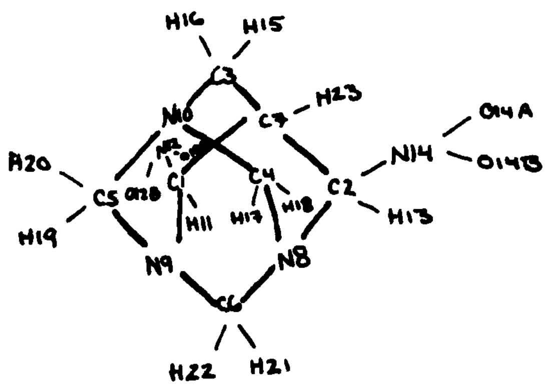
NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBF	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
1,2-DINITRO-7,8,9,10-TETRAAZAADAMANTANE (A,A) $C_6H_{10}N_6O_4$	74	1,081,493	1600.30	2936.87	40*



MOLECULE	NBF	#2E INT	2E INT	SCF	ITNS
1,2-DINITRO-7,8,9,10-TETRAAZAADAMANTANE(E,E) $C_6H_{10}N_6O_4$	74	1,007,307	1477.44	1335.35	19*



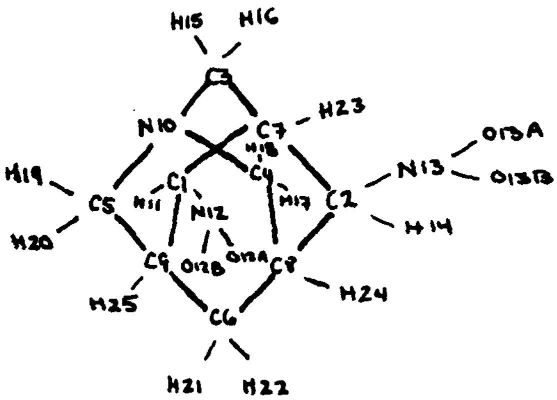
*1 x 10^{-6} A.U. CONV.

NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

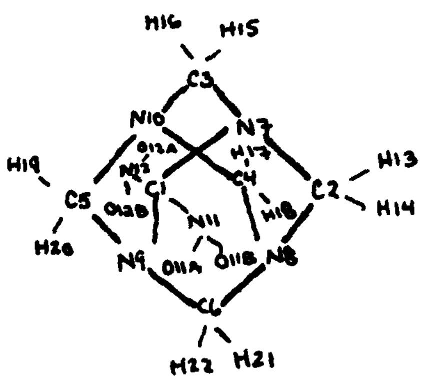
MOLECULE	NBF	#2E INT	TIMING(SECS) 2E INT	TIMING(SECS) SCF	ITNS
1,2-DINITRO-7,8,9,10-TETRAAZAADAMANTANE (E,A)	74	1,012,453	1477.37	1473.16	21*

$C_6H_{13}N_6O_4$



MOLECULE	NBF	#2E INT	TIMING(SECS) 2E INT	TIMING(SECS) SCF	ITNS
1,1-DINITRO-7,8,9,10-TETRAAZAADAMANTANE (A,E)	74	1,041,540	1510.67	1279.80	18*

$C_6H_{13}N_6O_4$



*1 x 10^{-6} A.U. CONV.

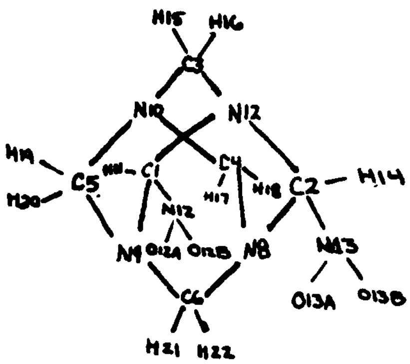
$C_6H_{10}N_6O_4$

NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

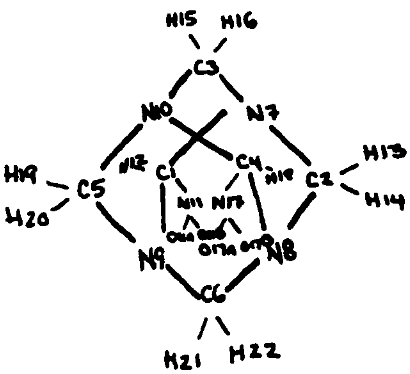
MOLECULE	NBF	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
1,2-DINITRO-7,8,9,10-TETRAAZAADAMANTANE (E,A)	74	1,012,453	1477.37	1473.16	21*

$C_5H_{10}N_6O_4$



MOLECULE	NBF	#2E INT	TIMING (SECS) 2E INT	SCF	ITNS
1,4-DINITRO-7,8,9,10-TETRAAZAADAMANTANE (A,E)	74	1,010,318	1460.35	1051.65	15*

$C_6H_{10}N_6O_4$

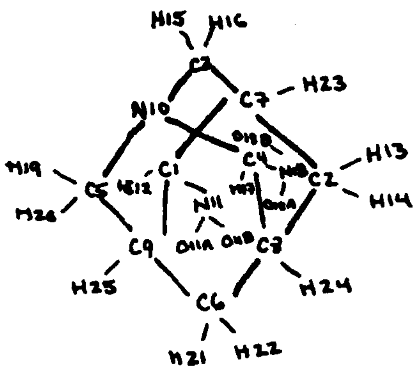


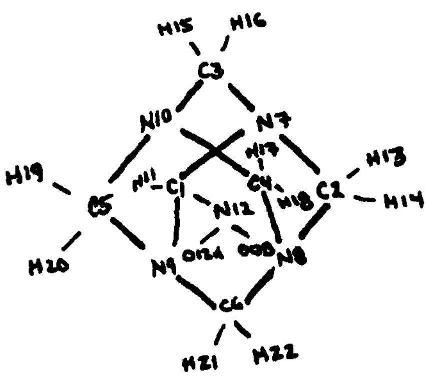
* 1×10^{-6} A.U. CONV.

NITROEXPLOSIVES

AB-INITIO, MODPOT/VRDDO

MOLECULE	NBE	#2E INT	TIMING(SECS)		
			2E INT	SCF	ITNS
1,4-DINITRO-7,8,9,10-TETRAAZAADAMANTANE (A,A) $C_6H_{13}N_6O_4$	74	1,361,395	1456.75	974.71	14*
1-NITRO-7,8,9,10-TETRAAZAADAMANTANE (E) $C_6H_{11}N_5O_2$	63	761,136	1048.93	831.44	16*





*1 x 10^{-6} A.U. CONV.

IV. Decomposition Pathways of Energetic Compounds

A. Ab-Initio SCF, GVB and MC-SCF/CI Calculations on HNO_2 and CH_3NO_2 as Prototypes of R-NO_2 Dissociation Pathways

In order to trace the decomposition pathways of energetic compounds it is necessary to go to beyond-the-SCF-Hartree-Fock method. There are several approaches [many-body perturbation-theory (MBPT) and/or coupled cluster or configuration interaction (CI)]. While each method has some advantages, however, at present if there is the possibility that multi-determinant reference states may be important then CI calculations are necessary to sort out the states.

Preliminary ab-initio SCF, GVB (generalized valence bond) and MC-SCF/CI (multiconfiguration SCF/configuration interaction) calculations were also carried out for the dissociation of HNO_2 (H--NO_2) as the prototype of R--NO_2 dissociation. The GVB calculations indicated and MC-SCF/CI calculations confirmed that HNO_2 like the isolectronic O_3 (for which in 1971 we had carried out very large scale ab-initio CI calculations) had a two configuration ground state. The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) at the equilibrium geometry and for a portion of the dissociation curves were π-orbitals located out of plane to the NO_2 group. At the equilibrium distance the ground configuration weight of 0.9160 $(\pi)^2$ and 0.4013 $(\pi^*)^2$ in the GVB calculation and 0.9106 $(\pi)^2$ and 0.3992 $(\pi^*)^2$ respectively in the MC-SCF/CI calculation which allowed all possible singlet combinations $\pi\rightarrow\pi^*$ and σ(H--NO_2)$\rightarrow\sigma^*$(H--NO_2) for all four molecular orbitals. This close correspondence of results from the two methods is very encouraging for the use of GVB as reliable preliminary screen for the necessity of multi-determinant reference states.

Part way out along the H--NO_2 dissociation curve the HOMO and LUMO became σ orbitals which were respectively bonding and anti-bonding between H--NO_2 and for proper dissociation this system also needs at least an additional two configurations corresponding to mixing of these σ and σ^* orbitals. Thus multideterminant reference states are a necessity to describe dissociation properly.

Preliminary calculations were carried out on localizing various combinations of molecular orbitals to see which ones might be suitable for tracing dissociation pathways. This is a new untested approach and much exploration and examination remains to be done.

To check whether this might be a general phenomenon for dissociation of R--NO_2 compounds we next carried out ab-initio SCF and GVB calculations on CH_3NO_2. The GVB calculations at the equilibrium distance indicated there was also mixing of the HOMO and LUMO where these orbitals were again π-like orbitals located out of plane to the NO_2 group and that

this system also had a two configuration ground state. At the equilibrium distance the coefficients of the two configurations were 0.9204 (π-like)^2 and -0.3909 (π^*-like)^2. Again for the dissociation of CH_3--NO_2, as with the dissociation of H--NO_2, part way along the CH_3--NO_2 dissociation curve the HOMO and LUMO changed character and became σ-like bonding and anti-bonding orbitals between the CH_3 and the NO_2 and again at least two additional configurations will now be necessary to describe properly the dissociating system.

These preliminary calculations on HNO_2 and CH_3NO_2 were carried out by Dr. Kaufman on a visit to NRC[2] (with collaboration of Dr. Michael Dupuis) and are being continued at the Johns Hopkins University.

To examine this mixing of configurations in more detail for these systems and for larger systems, the program is being enlarged at the Johns Hopkins University to handle more basis functions and also our ab-initio integral MODPOT/VRDDO/MERGE options will be meshed in with GVB and MC-SCF/CI programs to enable tractable calculations on large molecules.

B. Desirable New Strategies

The major bottleneck in any beyond-the-Hartree-Fock method on very large systems is the transformation from integrals over atomic orbitals to integrals over molecular orbitals. We have been implementing a large scale version of this step as well as exploring new strategies for this problem. A note on some of these new strategies, "Improved Strategies for Ab-Initio Computations on Large Molecules," was presented at the Texas Conference on Theoretical Approaches to Chemical Dynamics, Austin, Texas, March 1981 and at the International Sanibel Symposium on Atomic, Molecular and Solid State Theory, Palm Coast, Florida, March 1981. A note on this has been accepted for publication and is in press, in the Symposium Issue.

V. Other Program Development

We have been developing both software and programs for our Computer Automation Naked Mini and plotter. To plot our electrostatic molecular potential contour maps we have written special spline routines with tension to interpolate smoothly. We have also written software for our Naked Mini to communicate directly with the CDC since this will make an "intelligent" terminal capable of storing and manipulating data in addition to just data communicating as with ordinary terminals. We have also put our geometry generating programs on the Naked Mini. The instant turn around that this affords has been most valuable especially for the complicated cyclic ethers and large nitrocompounds.

VI. Lectures Presented on this Research (*Invited Lectures)

A. Lectures Presented at the following National or International Meetings: Joyce J. Kaufman.

* "Improved Strategies for Ab-Initio Computations on Large Molecules," Texas Conference on Theoretical Approaches to Chemical Dynamics, Austin, Texas, March 1981.

* "Ab-Initio MODPOT/VRDDO/MERGE Calculations and Electrostatic Molecular Potential Contour Maps for Mechanism of Cationic Polymerization," International Sanibel Symposium on Atomic, Molecular and Solid State Theory, Palm Coast, Florida, March 1981.

* "Ab-Initio Quantum Chemical Calculations Permit Prediction of Propensities of Substituted Cyclic Ethers to Polymerize," Division of Polymer Chemistry, 181st American Chemical Society National Meeting, Atlanta, Georgia, March 1981.

"Ab-Initio Quantum Chemical Calculations and Electrostatic Molecular Potential Contour Maps for the Mechanism of Cationic Polymerization," American Physical Society Meeting, Baltimore, Maryland, April 1981.

"Ab-Initio Quantum Chemical Calculations on Nitro Compounds," American Physical Society Meeting, Baltimore, Maryland, April 1981.

* "Ab-Initio Quantum Chemical Calculations on Large Molecules Using Improved Computational Strategies," NRCC Workshop on Effective Potential Methods in Quantum Chemistry, Los Alamos, New Mexico, June 1981.

"Ab-Initio Quantum Chemical Calculations on Large Molecules Using Desirable Computational Strategies," American Conference on Theoretical Chemistry, University of Colorado, Boulder, Colorado, June 1981.

B. Lectures Scheduled to be Presented at the Following National or International Meetings: Joyce J. Kaufman

* "Ab-Initio MODPOT/VRDDO/MERGE Calculations on Large Nitro-explosives," International Sanibel Symposium on Atomic, Molecular and Solid State Theory, Palm Coast, Florida, March 1982.

* "Ab-Initio Calculations and Partitioned Energy Contributions for Calculations on Crystals," International Sanibel Symposium on Atomic, Molecular and Solid State Theory, Palm Coast, Florida, March 1982.

"Ab-Initio Calculations on Large Nitrocompounds," Division of Physical Chemistry, American Chemical Society National Meeting, Las Vegas, Nevada, March 1982.

* "Ab-Initio MODPOT/VRDDO/MERGE Calculations on Large Nitrocompounds," 4th International Congress of Quantum Chemistry, Uppsala, Sweden, June, 1982.

C. Invited Lectures Presented at ONR or DOD Meetings

"Ab-Initio Quantum Chemical Calculations of the Decomposition of Energetic Materials and Their Subsequent Reactions," Workshop on Fundamental Research Directions for Decomposition of Energetic Materials (also was overall Chairman of the Section on Theoretical Aspects of Energy Transfer and Reactive Pathways), University of California, Berkeley, California, January 1981, Joyce J. Kaufman.

"Prediction of Polymerization Propensities of Energetic Substituted Ethers from Ab-Initio Quantum Chemical Calculations and Electrostatic Molecular Potential Contour Maps", Symposium on the Chemistry and Synthesis and Characterization of Energetic Monomers and Prepolymers, The Johns Hopkins University Applied Physics Laboratory, Columbia, Maryland, July 1981, P. C. Hariharan.

D. Other Trips Related to this Research Contract

1. At the request of our contract monitor Dr. Richard Miller, Dr. Kaufman visited SRI with him in January 1981 to interact on new developments in polymer propagation.

2. At the invitation of ARO, Dr. Kaufman participated in the meeting on High Energy Molecules, Their Synthesis and Reactions, Hilton Head, South Carolina, April 1981 as an expert on quantum chemical computational methods.

3. At the request of our contract monitor, Dr. Richard Miller, Dr. Walter S. Koski and Dr. P. C. Hariharan participated in the Symposium on the Chemistry and Synthesis and Characterization of Energetic Monomers and Prepolymers, The Johns Hopkins University Applied Physics Laboratory, Columbia, Maryland, July 1981, and in an informal technical exchange at ONR to discuss high density explosives research, July 1981.

VII. Papers on this Research

A. Accepted for publication, in press.

1. "Ab-Initio MODPOT/VRDDO/MERGE Calculations on Energetic Compounds. I. Mechanism of Initiation of Cationic Polymerization from Electrostatic Molecular Potential Contour Maps*," Frank L. Tobin, P. C. Hariharan, Joyce J. Kaufman, and Richard S. Miller. An invited paper presented at the International Sanibel Symposium on Atomic, Molecular and Solid State Theory, Palm Coast, Florida, March 1981. In press, Int. J. Quantum Chem., Symposium Issue.

*Paper XIII in the Series "Molecular Calculations With the Non-Empirical Ab-Initio MODPOT/VRDDO/MERGE Procedures."

2. "Symposium Notes: Additional New Computational Strategies for Ab-Initio Calculations on Large Molecules," Joyce J. Kaufman, P.C. Hariharan and Herbert E. Popkie. Part of an invited paper presented at the International Sanibel Symposium on Atomic, Molecular and Solid State Theory, Palm Coast, Florida, March 1981. In press, Int. J. Quantum Chem., Symposium Issue.

3. "Reliable Ab-Initio Calculations for Energetic Species," Joyce J. Kaufman. An invited lecture presented at the NATO Advanced Study Institute on Fast Reactions in Energetic Systems, Preveza Beach, Greece, July 1980. In press in the Proceedings

B. Already published

4. "Electrostatic Molecular Potential Contour Maps from Ab-Initio Calculations. 1. Biologically Significant Molecules. 2. Mechanism of Cationic Polymerization," Joyce J. Kaufman, P.C. Hariharan, F.L. Tobin and C. Petrongolo. An invited lecture presented at the 179th American Chemical Society National Meeting at the Symposium on Electrostatic Potentials in Biology and Chemistry. In CHEMICAL APPLICATIONS OF ATOMIC AND MOLECULAR ELECTROSTATIC POTENTIALS. REACTIVITY, STRUCTURE, SCATTERING AND ENERGETICS OF ORGANIC, INORGANIC AND BIOLOGICAL SYSTEMS, Eds. P. Politzer, and D.G. Truhlar, Plenum Press, New York, N.Y. 198], pp. 335-380.

VIII. Additional Information of Interest

Dr. Joyce Kaufman has just been elected a Membre Correspondant de L'Academie Europeenne des Sciences, des Arts et des Lettres, March 1981.

IX. Project Personnel

Joyce J. Kaufman, Ph.D., Principal Investigator

Frank C. Tobin, Ph.D.

The majority of the quantum chemical calculations on the energetic polymers were due to him.

P. C. Hariharan, Ph.D.

Development of the program for predicting crystal structure and testing of it.

Quantum chemical calculations on the nitrocompounds and energetic polymers.

Development of software and programs for the minicomputer.

Victor Lewchenko, Ph.D.

Joined our group recently. Working part time on the program for predicting crystal structure and testing of it.

W. Andrezj Sokalski

A visitor to our group who collaborated with the project on the development of the program for partitioning of the SCF energy into its various components.

ENERGETIC MATERIALS RESEARCH

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